

N-ButylNitrite  
544-16-1 | DTXSID8049418

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 74.8 °C

Global applicability domain: Inside

Local applicability domain index: 8.64e-01

Confidence level: 7.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N-Butylnitrite</div> <div>Measured: 78.0</div> <div>Predicted: 74.8</div>	<div>Image not found</div> <div>Isobutyl nitrite</div> <div>Measured: 67.0</div> <div>Predicted: 74.6</div>	<div>Image not found</div> <div>tert-Butyl nitrite</div> <div>Measured: 63.0</div> <div>Predicted: 74.7</div>
<div>Image not found</div> <div>3-Methylbutyl nitrite</div> <div>Measured: 105</div> <div>Predicted: 104</div>		